

What is claimed is:

1. Crystalline GFS.
2. The crystalline GFS of claim 1 wherein said GFS is *E. coli* GFS.
3. The crystalline GFS of claim 1 wherein said GFS is recombinant GFS.
4. The crystalline GFS of claim 1 wherein said GFS is crystallized with a co-factor selected from the group consisting of NADPH and NADP+.
5. The crystalline GFS of claim 1 wherein said GFS comprises the mature sequence of naturally-occurring GFS.
6. A crystalline composition comprising GFS in association with a second chemical species.
7. The composition of claim 6 wherein said second chemical species is selected from the group consisting of NADPH, NADP+ and a potential inhibitor of GFS activity.
8. A model of the structure of GFS comprising a data set embodying the structure of crystalline GFS of claim 1.
9. The model of claim 8 wherein said data set was determined by crystallographic analysis of GFS.

10. The model of claim 8 wherein said data set was determined by NMR analysis of GFS.

11. The model of claim 8 wherein said data set embodies the entire structure of GFS.

12. The model of claim 8 wherein said data set embodies a portion of the structure of GFS.

13. The model of claim 12 wherein said portion is the active site of GFS.

14. The model of claim 8 wherein said GFS is complexed with a second chemical species selected from the group consisting of NADPH, NADP+ and a potential inhibitor of GFS activity.

15. A computer system comprising computer hardware and the model of claim 8.

16. A method of identifying a species which is an agonist or antagonist of GFS activity or binding comprising: (a) providing the model of claim 8, (b) studying the interaction of candidate species with such model, and (c) selecting a species which is predicted to act as said agonist or antagonist.

17. A species identified in accordance with the method of claim 16.

18. A process of identifying a substance that inhibits GFS activity or binding comprising determining the interaction between a candidate substance and a model of claim 8.

19. A method of identifying inhibitors of GFS activity by rational drug design comprising:

(a) designing a potential inhibitor that will form non-covalent bonds with one or more amino acids in the GFS sequence based upon the crystal structure co-ordinates of crystalline GFS of claim 1;

(b) synthesizing the inhibitor; and

(c) determining whether the potential inhibitor inhibits the activity of GFS.

20. The method of claim 19 wherein said inhibitor is designed to interact with one or more amino acids in the GFS sequence selected from the group consisting of Arg12, Met14, Val15, Arg36, Asn40, Leu41, Ala63, Ile86, Gly106, Ser107, Ser108, Cys109, Tyr136, Lys140, Asn165, Leu166, His179, Val180, Leu184, Val201, Trp202, Arg209, and Lys283.

21 An agonist or antagonist identified by the method of claim 19.

22 A substance identified by the method of claim 18.

23. A method of identifying a species which is an agonist or antagonist of human FX protein or binding comprising: (a) providing the model of claim 8, (b) studying the interaction of candidate species with such model, and (c) selecting a species which is predicted to act as said agonist or antagonist.

24. A species identified in accordance with the method of claim 23.

25. A process of identifying a substance that inhibits human FX protein activity or binding comprising determining the interaction between a candidate substance and a model of claim 8.

26. A method of identifying inhibitors of human FX protein activity by rational drug design comprising:

(a) designing a potential inhibitor that will form non-covalent bonds with one or more amino acids in the GFS sequence based upon the crystal structure co-ordinates of crystalline GFS of claim 1;

(b) synthesizing the inhibitor; and

(c) determining whether the potential inhibitor inhibits the activity of human FX protein.

27. The method of claim 26 wherein said inhibitor is designed to interact with one or more amino acids in the GFS sequence selected from the group consisting of Arg12, Met14, Val15, Arg36, Asn40, Leu41, Ala63, Ile86, Gly106, Ser107, Ser108, Cys109, Tyr136, Lys140, Asn165, Leu166, His179, Val180, Leu184, Val201, Trp202, Arg209, and Lys283.

28. An agonist or antagonist identified by the method of claim 26.

29. A substance identified by the method of claim 25.